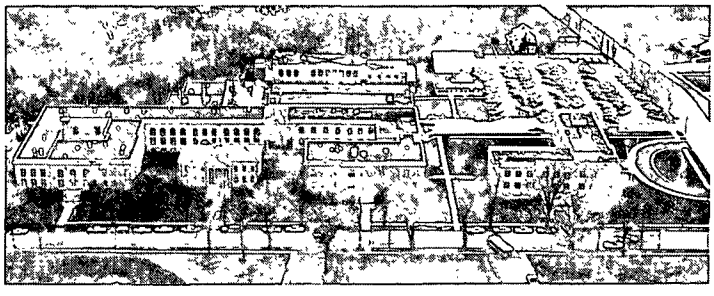

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REVERSE VARIABLE TECHNIQUE FOR THE SOLUTION OF SYSTEMS OF ODE'S AND ADE'S

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Reverse Variable Technique for the Solution of Systems of ODE's and ADE's

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ABSTRACT:

Although many numerical techniques have been developed to solve systems of ODE's, PDE's and ADE's, all assign the independent variable step, i.e., time, space, and compute the changes in dependent variables. On the surface, this appears to be the most reasonable approach. What would happen if the process were reversed and the dependent variables were manipulated and the change in independent variable determined? This is the basis of the reverse variable method which may provide a number of advantages over the standard techniques. The method is described and applied to solution of several standard stiff and non-stiff ODE's. Extensions of the method to PDE's, ADE's and even to determining roots of algebraic equations are discussed.

INTRODUCTION:

With the wide variety of numerical techniques available to solve ODE's, it hardly seems possible that yet another technique could be found. Despite this, the recent literature has seen a flowering in this area (Byrne et. al., Hanna)

Although the methods differ in detail, they all fundamentally assume or determine a change in the independent variable, dt, and compute the changes in dependent variables, y. What would happen if instead, the procedure were reversed.

For a single equation where f is not a function of t,

$$dt = dy/f(y) \qquad \ldots\ldots\ldots (1)$$

$$t = \int dy/f(y) \qquad \ldots\ldots\ldots (2)$$

A variety of well-known integration techniques are available to approximate t. This approach is quite useful for integration of high-order kinetics which occur in bleaching or extraction of wood fibers. Such reactions are usually limited by component concentrations rather than by reactor residence time. Simpson's rule proved to be very time consuming and occasionally unstable in solving these equations. The solution to the problem was to integrate piece-wise on the controlling reactant, a,

$$dt = - dC_a/R_a(C_1,\ldots,C_a,\ldots) \qquad \ldots\ldots\ldots (3)$$

$$t = 0 \qquad C_a = C_a^0$$

$$\Delta t^i = t^{i+1} - t^i = \frac{C_a^i - C_a^{i+1}}{R_a(C_a^{i+1/2})} \qquad \ldots\ldots\ldots (4)$$

where R is evaluated at the half-interval. C_a is incremented based on C_a^0. The advantage is provided by an accurate estimation of R_a at each interval. For R having a power law form,

$$R_a = k\, C_a^p C_b^q \ldots C_n^z \qquad \ldots\ldots\ldots (5)$$

and C_b, .. related to C_a through algebraic relations,

$$C_b = g_b(C_a) \qquad \ldots\ldots\ldots (6)$$

the time step is computed piece-wise semianalytically.

$$\Delta t^i = (1/C_a^{(i+1)(p-1)} - 1/C_a^{i(p-1)})/K^i \qquad \ldots\ldots\ldots (7)$$

where $p \neq 1$, $C_a^0 \neq 0$ and $K^i = (p-1)\, k\, C_b^{iq} C_c^{ir} \ldots$.

This is the most common situation and the method is therefore quite useful for a variety of reactions. The concentration of the key reactant is reduced, the concentrations of other reactants are evaluated at the half-interval though

the stoichiometric relations and R is evaluated at the half interval. If one of the components is limiting, the concentrations are determined by interpolation and the integration is stopped. If t^{i+1} exceeds the reactor space time, the actual time available is assumed and (7) is inverted to compute C_a^{i+1}.

This method is very rapid, accurate and simple for the types of reactions in this category. The method works regardless of the order of the reaction. Zero and first order reactions are integrated to different solutions. The reaction rate is accurately known at each iteration.

Although the method is only second order in the prediction of t^{i+1}, the error accumulation is less than could occur with any traditional approach.

For multivalued problems, the reverse-variable approach also tends to find nontrivial solutions if they exist. This is illustrated easily by solving the following simple example.

$$y' = \sqrt{y} \qquad y(0) = 0 \qquad \text{.....(8)}$$

The exact non-trivial solution, $y = t^2/4$ and R-V solution obtained by Eq. 4, were obtained for $\Delta y = 0.1$ and 0.01 respectively. Euler-based methods fail to find the non-trivial solution for this problem because both the initial value and slope are zero.

For each case, the absolute error in t increases to .19 and .06, respectively, at the first iteration and then remains constant for all subsequent iterations. The relative error rises initially and then decreases rapidly to zero. Thus the numerical solution can be represented by the following

$$y = (t - \epsilon)^2/4 \qquad \text{.....(9)}$$

for all time where ϵ = 0.19 and .06, respectively.

This absense of error growth occurs because f(y) is known for any y with an accuracy which is independent of t. This property applies to more arbitrary systems of equations but the statement that the error does not increase cannot be made unequivocably. It should be noted that the piece-wise semianalytic approach of Eq.7 provides the exact solution.

Because the solution diverges, in a sense, Δt decreases from .01 to .0014 over the course of the solution for Δy = .01.

This method is faster and more stable than Gear's method for extremely rapid reactions. For the following hypothetical reaction,

$$y' = -k\, y^5\, z^{0.5} \qquad \text{.....(10)}$$

$$z' = 0.5\, dy/dt \quad \text{or} \quad z = z^0 + 0.5\, \Delta y \qquad \text{.....(11)}$$

where

$$k = 100 + 1 \times 10^5\, e^{1/y}$$

$y(0) = 1 \quad z(0) = 10$

A comparison of the R-V method with Gear is shown in Table I.

Table I

R-V Method				Adams-Bashford (DGEAR, IMSL)		
y	Iteration	t	k'*	Iteration	t	k*
1	1	≃ 0	.34	19	≃ 0	.027
0.9	2	≃ 0	.38	6	≃ 0	.031
0.8	3	≃ 0	.44	7	≃ 0	.035
0.7	4	≃ 0	.52	6	≃ 0	.041
0.6	5	≃ 0	.66	6	≃ 0	.051
0.5	6	≃ 0	.92	7	≃ 0	.076
0.4	7	≃ 0	1.5	6	.00001	.114
0.3	8	≃ 0	3.5	6	.00001	.247
0.2	9	≃ 0	18	6	.00002	1.47
0.1	10	.0001	2700	95	.00002	22.7
0.0008	11	.0001	2700	95	.00002	2.5×10^{47}

* k or $k'(= k z^{0.5}) \times 10^{-7}$

The results are somewhat surprising in that they show that time is limiting. The R-V method handles the very high rate with no problem while the Adams-Bashford method (IMSL) becomes oscillatory and eventually fails. The rate constant k varies from 0.027 to 2.5×10^{47}. In addition the A-B method required 259 iterations compared to 11 for R-V.

When y changes rapidly, time steps are computed to be small and as y nears depletion, time steps increase. Reaction of the last increment of y requires only a single iteration while fixed step methods may require orders of magnitude more iterations.

The advantage of a semi-implicit or semianalytic approach may be obvious for a single ODE or ADE but how could such an approach be generalized to multiple ODE's? Could the method be used to solve ADE's, PDE's or other types of equations?

Generalized Reverse-Variable Method

For N ODE's,

$$y_i' = f_i(y_1, \ldots y_i, \ldots y_n, t, f_j) \quad i = 1,n \qquad \ldots\ldots\ldots\ldots\ldots (12)$$

where j is not equal to i and $y_i = y_i^0 \quad t = 0$.

Begin by assigning Δy_i^n where n refers to iteration n. For nonzero initial values assign

$$\Delta y_i^n = |y_i^0/NY| \qquad \ldots\ldots\ldots (13)$$

where NY is a single integration parameter for all y_i. When $y_i^0 = 0$ assign

the increment an arbitrary value 1/NYO where NYO is chosen independently. Next compute,

$$\Delta t_i^n = \Delta y_i^n / f_i \qquad \text{.....(14)}$$

where f_i is evaluated at the half interval,

$$y_{i+1/2}^n = (y_i^{n-1} + y_i^n)/2 \qquad \text{.....(15)}$$

and

$$y_i^n = y_i^{n-1} + \Delta y_i^n \qquad \text{.....(16)}$$

and t and f_j are evaluated at the last iteration, t^{n-1}, f_j^{n-1}.

Next the slopes must be consistent with positive Δt_i^n for all i. For any i for which $\Delta t_i^n < 0$, the sign of Δy_i^n is reversed and f_i^n and Δt_i^n are reevaluated.

If after reevaluation Δt_i^n is negative, this indicates a rapid change in slope of the function over the increment. In this case, the increment Δy_i^n is reduced and the temporary value of y_i^n is evaluated at the new half-interval. This is repeated until all time increments are positive. If this is repeated several times, the algorithm interprets this as a steady function and this variable is considered to be at a pseudo-steady state over this increment.

The actual time increment is chosen as the minimum of the set of Δt_i^n.

$$\Delta t^n = \min \Delta t_i^n \qquad \text{.....(17)}$$

Each increment Δy_i^n is rescaled by the ratio of the minimum time increment and Δt_i^n.

$$\Delta y_i^n = \Delta y_i^n \frac{\Delta t^n}{\Delta t_i^n} \qquad \text{.....(18)}$$

Time is incremented by the minimum time step,

$$t = t + \Delta t_n \qquad \text{.....(19)}$$

Rescaling results in a progression in step sizes which decrease with decreasing f_i. The equation with the highest eigenvalue determines the time scale for each step. The dominant equation can vary with each iteration and the time scale will vary in a corresponding fashion.

Special conditions in which the slope is repeatedly zero are also handled. When $f_i^n = 0$, that time increment is ignored and y_i is not incremented. If $\min \Delta t^n = 0$, then a pseudo-steady state is assumed for all dependent variables and time is incremented by a user-specified amount.

ADVANTAGES

For many types of problems the R-V method is not much more difficult to implement than Euler's method and is no more storage intensive than any second order method. The method is most applicable to functions which are not strongly dependent on t. Stiffness is handled automatically through the rescaling. However, the efficiency drops for highly nonstiff systems due to the extra rescaling loop. Difficulties with most methods, which are avoided with the R-V method, are in choosing the optimal tolerance, initial time step and in some cases determining whether to evaluate the Jacobian.

Applications

The method has been applied to a wide variety of test problems designed to demonstrate strength or weakness in the approach. The various test problems are classified in Table II.

Table II

Stiff ODE's

- Robertson Problem
- Van der Poel equation (Norsett)
- Algebraic-Differential Equations, ADE's
- Ramp functions, discontinuous slopes (Norsett)
- Bleaching kinetics (Jones (1987, 1988)
- Oscillatory problem with stability implication (rigid undamped pendulum)
- Furnace control problem (Norsett)

Partial Differential Equation:

- 1-D transient heat conduction in a slab

Algebraic Equations, AE's:

- Three transcendental algebraic equations (Burden)

All examples were solved in a 286 IBM PC compatible in Fortran 77 compiled with a Microsoft 4.1 compiler. All variables were declared single precision. All but two of these are discussed below.

Stiff ODE's

Case 1 is the classic autocatalytic reaction (Robertson Problem).

$$y_1' = -0.04\, y_1 + 10^4\, y_2\, y_3 \qquad \text{.....(20)}$$

$$y_2' = 0.04\, y_1 - 10^4\, y_2\, y_3 - 3\, 10^7\, y_2^2 \qquad \text{.....(21)}$$

$$y_3' = 3\, 10^7\, y_2^2 \qquad \text{.....(22)}$$

$$y_1(0) = 1,\ y_2(0) = 0\ ,\ y_3(0) = 0$$

Comparisons of solutions at t = 10 and relative execution times for a variety of methods are reported by Davis (1984). This problem requires either an analytic or numerical Jacobian for successful solution by DGEAR. The R-V solved the problem in about 60 minutes including data transfer on a 286 PC.

For NY = 5000 and NY0 = 10000 this case was integrated to t = 10 in 800 iterations. Results are as shown in Figure 1. At t = 10, y_1 = .829, y_2 = 1.652 x10^{-5}, y3 = .1513 compared to the "EXACT" solution values of Caillaud and Padmanabhan reported by Mason, y_1 = .841, y_2 = 1.62 x10^{-5}, y_3 = .159. Differences could be attributed to use of single-precision variables.

Figure 1 here

Van der Poel Problem:

$$y_1' = -y_2 \qquad \text{.....(23)}$$

$$y_2' = -y_1 + 100\ (\ 1 - y_1^2)\ y_2$$

$$y_1(0) = 2 \quad y_2(0) = 0 \quad t \in [0,100]$$

For this problem, which is discussed by Norsett (1985), NY = 1 x 10^5, NY0 = 1 x 10^4. y_1 and y_2 are virtually zero over nearly the entire interval except in the immediate vicinity of t = 80.98. Y_1 drops rapidly to -133.7 and returns to zero as shown in Figure 2. The results agree with those reported by Norsett for several methods. The computed time step begins near 0.003 drops to 8 x10^{-8} when y_1 is -17.67 on the far side of the minimum in y_1 and increases again to .0026.

Figure 2 here

Undamped Pendulum Problem:

For a rigid undamped pendulum whose length is equal to g, Newton's Law reduces to

$$y_1' = y_2 \qquad \text{.....(24)}$$

$$y_2' = -\sin(y_1)$$

$$y_1(0) = \pi \quad y_2(0) = 0$$

The damped version of this equation poses no problems for most methods such as fourth order RK (stiff or nonstiff). These methods experience problems for zero damping and for the above initial conditions. For zero damping, Runga-

Kutta methods predict that the pendulum will go "over the top" indefinitely after two or three cycles even when $y_1(0)$ is as low as 3.1. The solution is supposed to exhibit continuous oscillation from 12 o'clock and not go over the top.

The R-V method solved the above problem for $y_1(0) = 3.141$, $y_2 = 0$ and NY = NYO = 30. A stiff fourth-order R-K algorithm was unstable for this initial condition. Because the initial condition cannot be set precisely at π, the solution is not expected to oscillate indefinitely. For the conditions used, the solution was slightly damped and oscillations continued but with a very slight drop off in amplitude over many oscillations. The position and velocity are shown in Figure 3 over five cycles up to t = 250.

Figure 3 here

ODE's with discontinuities (the simple furnace control problem)

$$y' = \begin{cases} y & \text{if status} = 0 \\ -y/2 & \text{if status} = 1 \end{cases} \qquad x \in [0,10] \qquad \ldots\ldots(25)$$

$$\text{with} \quad y(0) = 1 \text{ and } g(x,y) = \begin{cases} y - 2 & \text{if status} = 0 \\ y - 1 & \text{if status} = 1 \end{cases}$$

and

status = 0 initially
status is reset to 0 if $g(x,y) \leq 0$ and status = 1
status is reset to 1 if $g(x,y) \geq 0$ and status = 0

The R-V method solved the above problem and other problems with logic and discontinuous slopes to give the same results as the analytical solutions. The results for the furnace problem are shown in Figure 4 (NY = 100, iterations 984, execution time less than 2 seconds).

Figure 4 here

Differential Algebraic Equations

Given $y' = f(t,y,z)$ .....(26)

$0 = g(t,y,z)$ .....(27)

The approach recommended by Norsett is to take the total derivative of g (provided the partials are nonsingular) and solve the resulting set of ODE's as follows.

$$0 = \frac{\partial g}{\partial t} + \frac{\partial g}{\partial y} f + \frac{\partial g}{\partial z} z' \qquad \ldots\ldots(28)$$

This approach worked using the R-K method on the following ADE.

$$y' = - y + z \qquad \text{.....(29)}$$

$$0 = y^2 - 1 + z$$

$$y(0) = 1 \quad z(0) = 0$$

Applying the total derivative and solving for z',

$$z' = -2\, y\, y' \qquad \text{.....(30)}$$

This problem is interesting because it has multiple solutions. It also exhibits properties similar to optimization problems in which the algebraic equation acts as an equality constraint.

One solution [0.6155,0.6155] for large time is obtained with the above initial conditions. The other is [-1.615,-1.615]. It is interesting that y(0) = 0 and z(0) = 1 also gives the same first steady state solution. The R-V method tended to go to the first solution rather than the second. It was even more interesting that for a wide variety of initial conditions, the solution converged to the first steady state rather than the second.

Partial Differential Equations

A rather simple problem, that of unsteady one-dimensional heat conduction, is solved by discretizing the PDE in the spatial dimension, y. The dimensionless form of the equation is,

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \eta^2} = \frac{\theta_{i+1} - 2\,\theta_i + \theta_{i-1}}{\Delta \eta^2} \qquad \text{....(31)}$$

$$i = 2, N-1$$

$$\theta_1 = \theta_1(t), \quad \theta_N = \theta_N(t), \quad \theta_i(0) = 1.$$

where $\theta = (T_0 - T)/(T_1 - T_0)$, $\tau = \alpha t/b^2$ and $\eta = y/b$, b is the slab half-thickness, t is time, y is the spatial dimension and α is the thermal diffusivity. This problem is easily solved with the R-V method for steady boundary conditions, $\theta_1 = \theta_N = 1$ with N = 12, NY = NYO = 100 over the range τ = [0,1].

A comparison of the results with the analytical solution in Table II shows that the R-V solution is reasonably accurate over the entire range of space and time. Accuracy could be improved by defining variables as double-precision.

Table II

COMPARISON OF SOLUTION OF 1-D HEAT CONDUCTION PROBLEM WITH ANALYTICAL SOLUTION (Bird et. al. 1960)

τ	Y/b	θ ANALYTICAL	R-V
.0100	.8182	.8014	.7700
.0100	.6364	.9899	.9697
.0100	.4546	.9999	.9972
.0100	.2728	1.0000	.9998
.0100	.0910	1.0000	1.0000
.0400	.8182	.4796	.4800
.0400	.6364	.8014	.7916
.0400	.4546	.9462	.9346
.0400	.2728	.9899	.9834
.0400	.0910	.9986	.9960
.1000	.8182	.3156	.3172
.1000	.6364	.5835	.5816
.1000	.4546	.7762	.7713
.1000	.2728	.8916	.8850
.1000	.0910	.9432	.9360
.2000	.8182	.2228	.2260
.2000	.6364	.4252	.4267
.2000	.4546	.5901	.5901
.2000	.2728	.7056	.7044
.2000	.0910	.7648	.7629
.4000	.8182	.1337	.1382
.4000	.6364	.2566	.2607
.4000	.4546	.3586	.3623
.4000	.2728	.4316	.4350
.4000	.0910	.4697	.4729
.6000	.8182	.0816	.0870
.6000	.6364	.1566	.1623
.6000	.4546	.2189	.2248
.6000	.2728	.2635	.2696
.6000	.0910	.2868	.2929
1.0000	.8182	.0304	.0357
1.0000	.6364	.0584	.0639
1.0000	.4546	.0816	.0874
1.0000	.2728	.0982	.1042
1.0000	.0910	.1069	.1129

There is no reason why the approach could not be used for the solution of a variety of problems involving multidimensional PDE's such as that described recently by Byrne (1988). Currently, the method is being used to solve the Navier-Stokes equations for entrance flow in a 2-D duct.

Algebraic Equations

The method used to solve a limited class of algebraic equations is admittedly experimental. Intuitively, the solution of a set of algebraic equations is the steady state solution of a set of differential equations. For two equations and two unknowns,

$$0 = g_1(y_1, y_2) \quad \text{.....(32)}$$

$$0 = g_2(y_1, y_2) \quad \text{.....(33)}$$

the roots can be determined as the steady state solutions of

$$y_1' = g_1 \qquad y_1(0) = \text{arbitrary starting point} \quad \text{....(34)}$$

$$y_2' = g_2 \qquad y_2(0) = \text{arbitrary starting point} \quad \text{....(35)}$$

The R-V method is a type of multidimensional search which lends itself to this approach. Time is introduced as a dummy variable. Solutions of the following equations were obtained for a variety of starting points (Burden et. al. 1981):

$$y_1 + e^{(y_1 - 1.0)} + (y_2 + y_3)^2 - 27.0 = g_1 \quad \text{.....(36)}$$

$$e^{(y_2 - 2.0)/y_1} + y_3^2 - 10.0 = g_2 \quad \text{.....(37)}$$

$$y_3 + \sin(y_2 - 2.0) + y_2^2 - 7.0 = g_3 \quad \text{....(38)}$$

The order of the derivatives may affect the roots that are found. However, this property was not investigated thoroughly. One known solution is [1.0,2.0,3.0]. Other solutions were obtained by choosing various starting points as summarized in Table III. A steady state was assumed when dummy variable "time" exceeded 10.

Table III

Starting Points	Roots
0.1,0.1,0.1	4.13,3.032,-3.053
1.2,2.2,3.2	4.05,-1.80,3.153
1.5,1.5,1.5	4.13,3.027,-3.050
2.0,2.0,2.0	4.13,3.052,-3.053
5.0,5.0,5.0	4.048,-1.797,3.165
-5.0,-5.0,-5.0	no roots found (no steady state)
10,10,10	no roots found (no steady state)

In the above example, it was not known how many roots actually exist. There appear to be at least three real roots, [1,2,3], [4.05,-1.80,3.15], [4.13,3.03,-3.05], all within the range -5 to + 5. It is interesting that the

starting points needed to be very close to [1,2,3] in order for the method to converge to that root. This indicates that the root may be unstable in some sense. Judging by this it appears that of the three roots two are stable and one is unstable. The occurence of an odd number of real roots in which an odd number are unstable is frequently observed in reaction engineering problems.

As the method converges to a root, the minimum "time" step increases dramatically to 50 or more. As the method diverges the "time" step decreases to 10^{-8}. This suggests that a stopping criteria could be based on some choice of a minimum time step for divergence and maximum "time" for convergence to a root. A new set of starting points would be chosen automatically using a random seed. The method can also be used to solve for roots of complex variable equations by applying it to each of the real and imaginary parts.

Source Code:

Those interested in obtaining an annotated listing of the rather brief source code may contact the author at The Institute of Paper Chemistry.

CONCLUSIONS

More study may be necessary to determine the full range of applicability, to make in-depth comparisons with established techniques and to establish the limitations and advantages. The exact nature of the truncation error must be established. A way of solving simple optimization problems with this method has so far eluded the author.

The technique offers several advantages: simplicity, accurate derivative evaluations, limited or nonexistant error propagation, greater stability and automatic step size determination and tends to find nontrivial solutions. In some cases it may even be faster than some other methods. The method outlined displayed some interesting properties and may indeed be preferable to some methods for the solution of a variety of equations. This appears to be particularly true of the types of kinetics which initially provided the motivation for this work.

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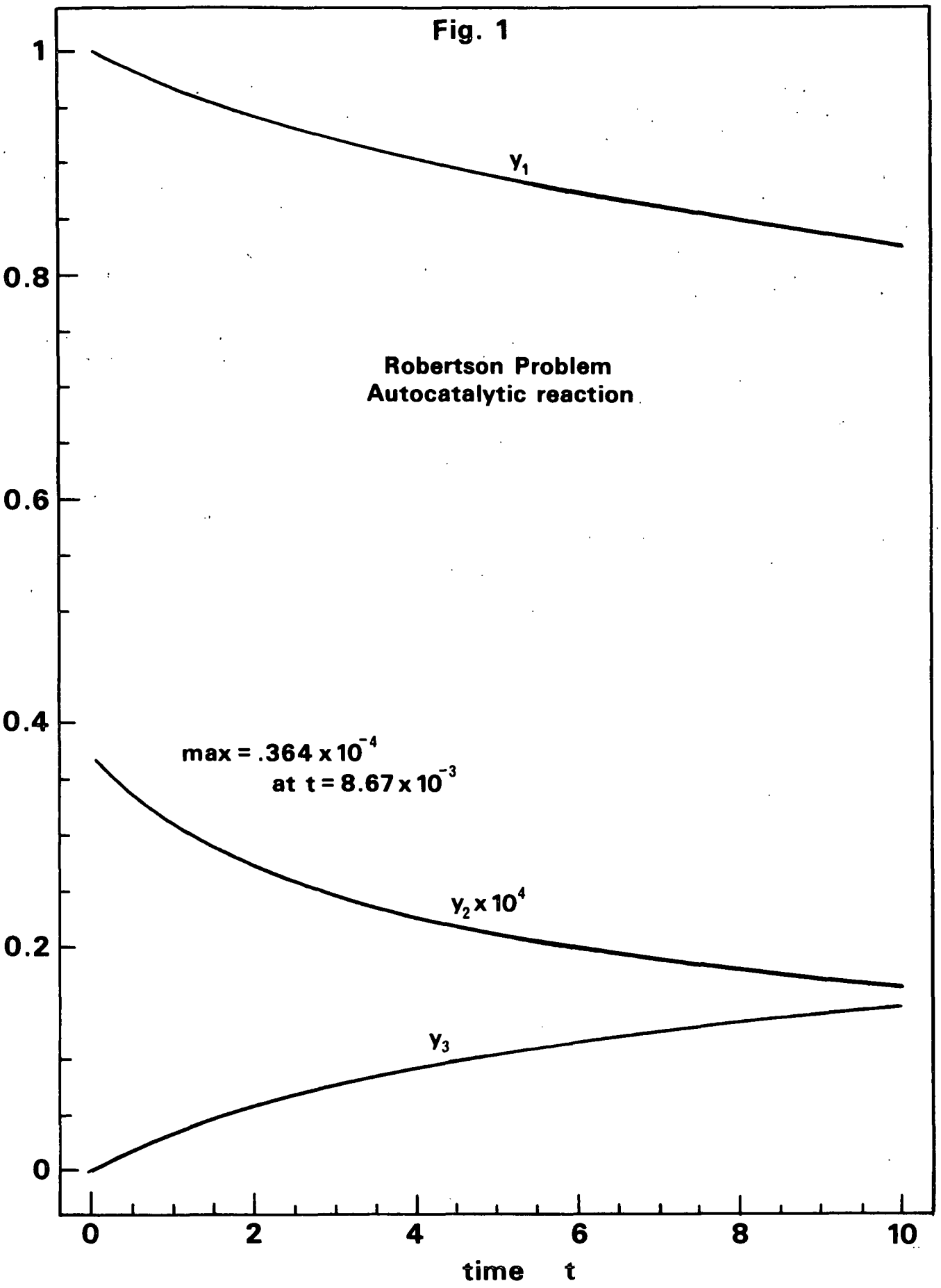


Fig. 1
1
0.8
0.6
0.4
0.2
0
y_1
Robertson Problem
Autocatalytic reaction
max = .364 x 10^{-4}
at t = 8.67 x 10^{-3}
$y_2 \times 10^4$
y_3
0
2
4
6
8
10
time t

Fig. 2

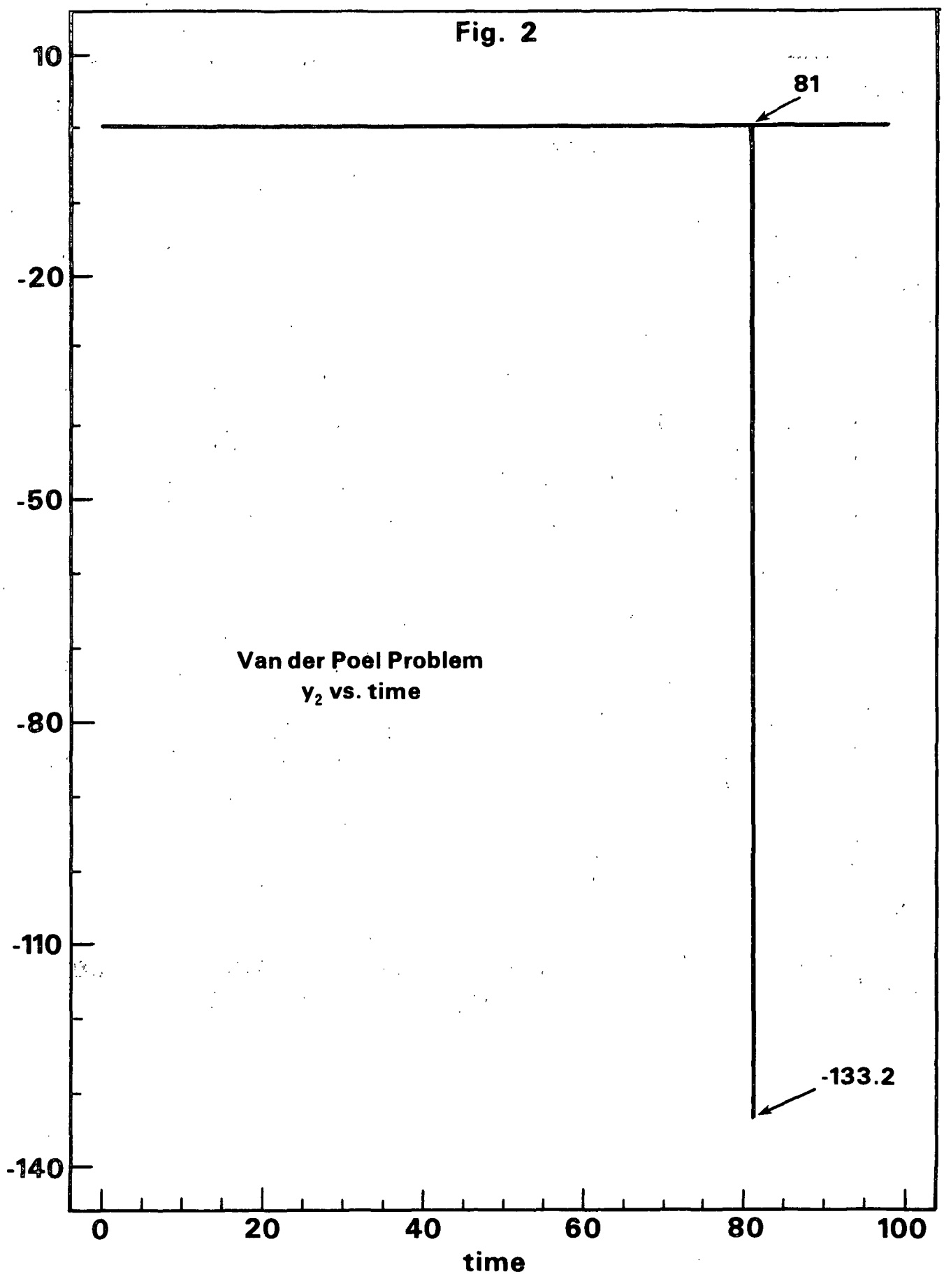
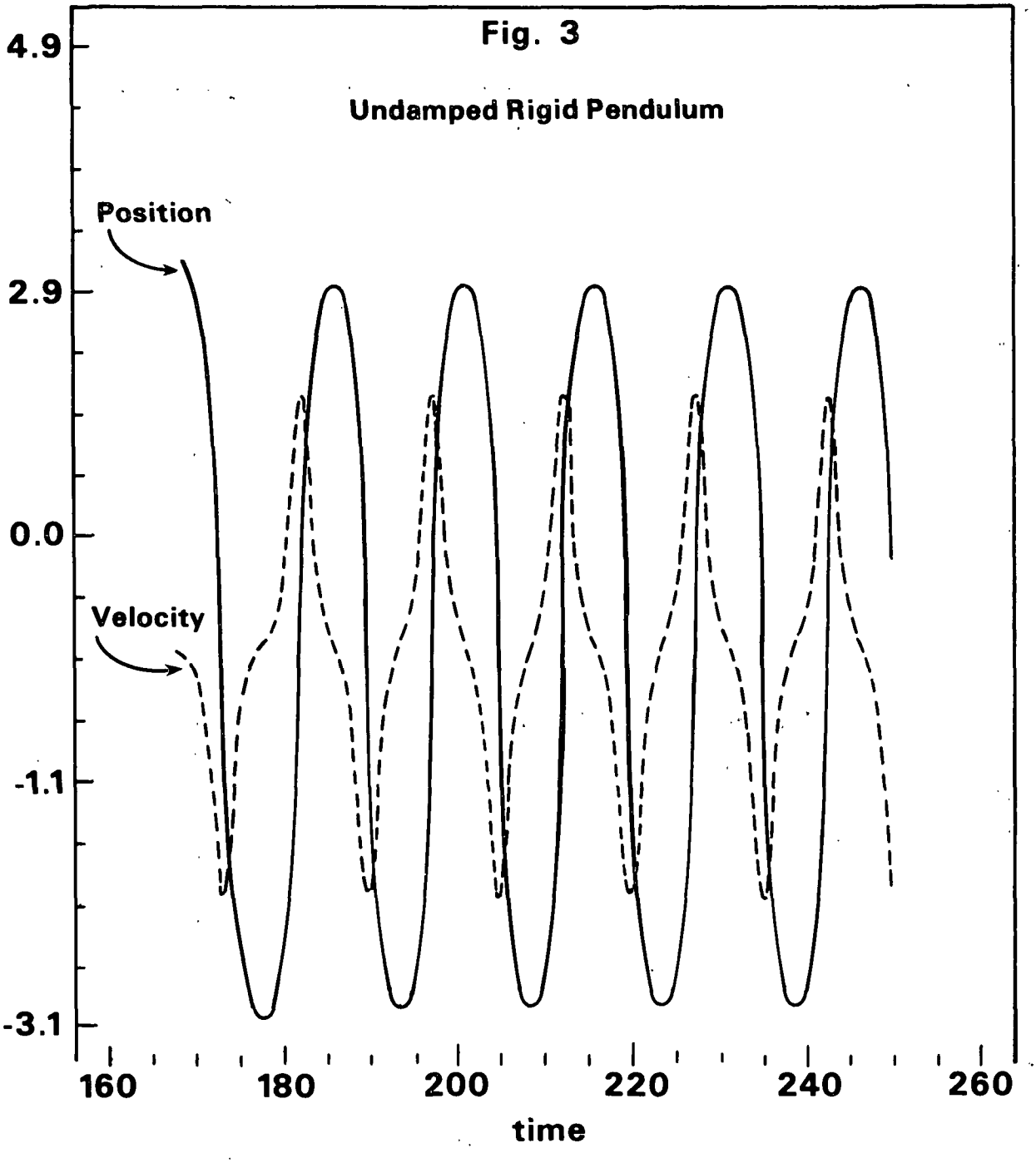

10
-20
-50
-80
-110
-140
81
-133.2
Van der Poel Problem
y_2 vs. time
0
20
40
60
80
100
time

Fig. 3


Undamped Rigid Pendulum
Position
Velocity
4.9
2.9
0.0
-1.1
-3.1
160
180
200
220
240
260
time

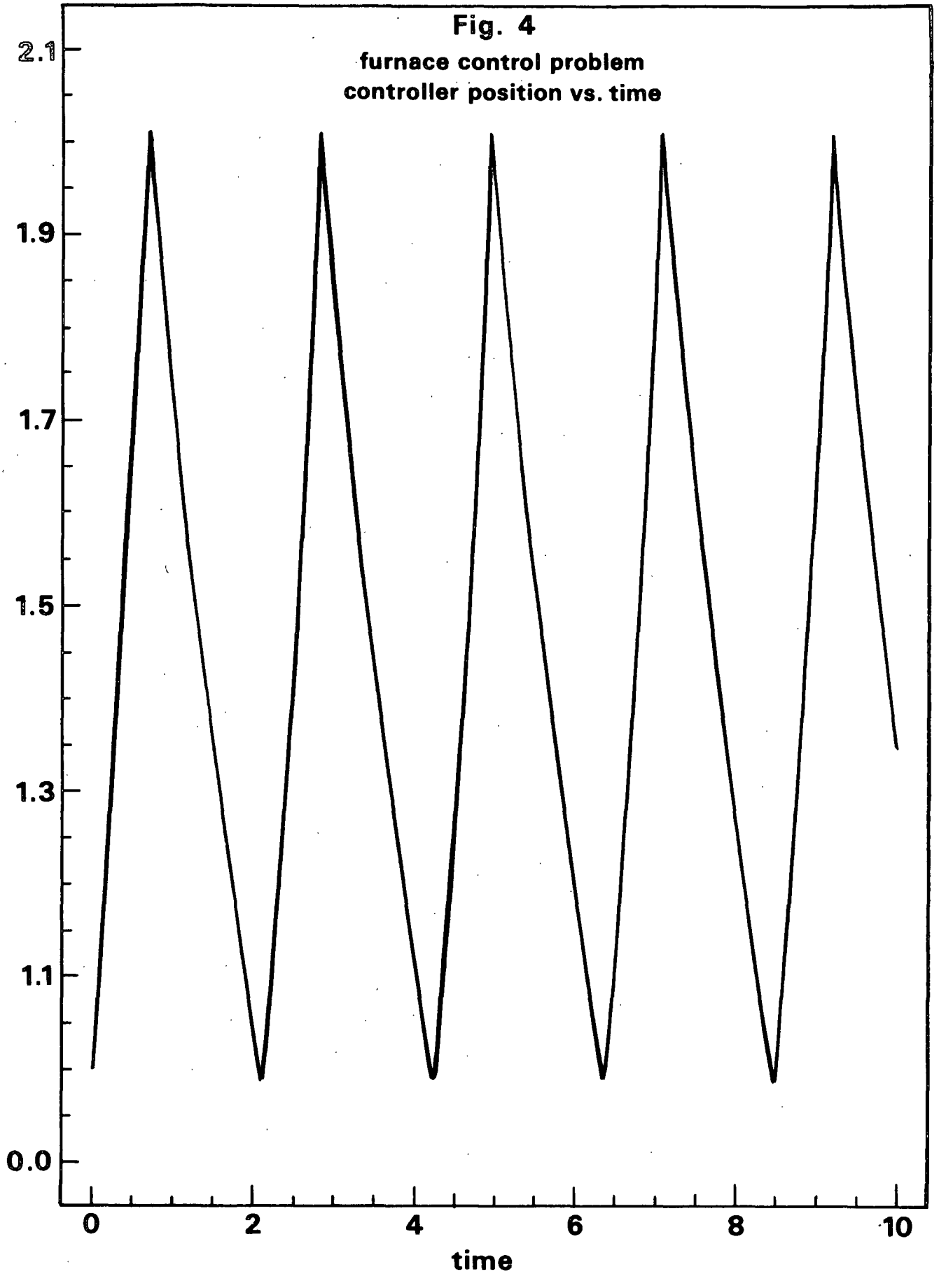


Fig. 4
furnace control problem
controller position vs. time
2.1
1.9
1.7
1.5
1.3
1.1
0.0
0
2
4
6
8
10
time